INSTITUTE FOR COMPUTATIONAL MATHEMATICS AND APPLICATIONS

Technical Report ICMA-89-143

November 1989

DIFFERENTIAL-GEOMETRIC TECHNIQUES FOR SOLVING DIFFERENTIAL ALGEBRAIC EQUATIONS

by

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1. Introduction

Differential-algebraic systems of equations (DAEs) arise in many areas of science and engineering. In particular, the equations of motion for a constrained mechanical system considered in this volume are usually modelled as a second order DAE. In recent years the literature on the numerical solution of such systems has grown rapidly, ~~(see e.g. the monographs~~ [1], [4]). However, up to now, existence theories for nonlinear DAEs are available only for a few selected classes of systems.

In [10] a differential-geometric approach was introduced for the analysis of the solution properties of a class of linear DAEs, and in [12] this approach was extended to general, semi-implicit, nonlinear equations of first and second order; that is, to systems with separated algebraic and differential equations. Moreover, it was shown there that these results lead to a general local parametrization approach for the computational solution of these systems.

The differential-geometric approach is based on the observation that, as long as we expect the solution of a DAE to be some smooth path in the space of dependent variables, the system must define a dynamical system in suitable subsets of that space. While this connection with dynamical systems is obvious for ordinary differential equations (ODEs), the same is certainly not true for DAEs. In fact, besides [10], [12] we are only aware of [9] as the only

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further study that specifically addresses this connection.

This article is intended to be an introductory overview of certain of the cited differential-geometric results and of some of the numerical algorithms that can be developed from them. In order to make the presentation widely accessible, we begin in section 2 with a brief summary of concepts and notations about sub-manifolds of finite-dimensional spaces and their first and second tangent bundles. Then section 3 presents an overview of basic results about dynamical systems in the form needed for our DAE-theory. This is followed in sections 4 and 5 by a presentation of the principal results of [12] on the existence and uniqueness of solutions and the use of local parametrizations. However, in order to avoid some of the technical aspects of the general theory we restrict ourselves, for the most part, to DAEs with certain linearity properties including, in particular, the equations of motion for constrained mechanical system mentioned earlier. In section 6 we discuss the computational implementation of local parametrizations and identify two useful parametrizations induced by the tangent space of the constraint manifold and by a so-called "coordinate partitioning", respectively. Then section 7 presents algorithms based on the application of explicit and implicit multi-step methods to the resulting local dynamical systems and in section 8 versions of these algorithms for the solution of the Euler-Lagrange equations are formulated. These algorithms generalize those previously discussed in [5] and [8]. Finally, in section 9 we give some computational results for a four-bar-linkage mechanism. .

2. Differential-Geometric Background

In this section we collect some basic material needed throughout the remainder of the presentation. For further details we refer to standard text on differential geometry such as [6] or [13].

We begin with some standard terminology. If U is an open set of R^n then a mapping $F:U \rightarrow R^m$ from U into R^m is of class C^ρ , $\rho \geq 0$, on U if all partial derivatives of F up to and including order ρ exist and are continuous in U.

More generally, on an arbitrary set S of R^n a map $F:S \to R^m$ is of class C^p if for each $x \in S$ there exists an open set $U \subset R^n$ containing x and a mapping $G:U \to R^m$ of class C^p that coincides with F throughout $U \cap S$. A map $F:S \to T$ between the sets $S \subset R^n$ and $T \subset R^m$ is a homeomorphism if F is a one-to-one mapping from S onto T and both F and its inverse $F^{-1}:T \to S$ are continuous. A homeomorphism $F:S \to T$ is a C^p-diffeomorphism between S and T and both F and F^{-1} are of class C^p.

As usual, $L(R^n,R^m)$ is the space of all linear mappings with domain R^n and range in R^m and by $L^2(R^n,R^m)$ the space of all bilinear maps from R^n to R^m. For any C^1-map $F:U \subset R^n \to R^m$, the derivative of F at $x \in U$ is the linear map DF(x) in $L(R^n,R^m)$ defined by $DF(x)h = \lim_{t\to 0} [F(x+th) - F(x)]$. In other words, DF(x) is the linear map that corresponds to the $m \times n$ matrix of first partial derivatives of F at x. Analogously, if F is of class C^2, then the second derivative of F at x is the bilinear map $D^2F(x) \in L^2(R^n,R^m)$ defined by the second partial derivatives of F at x. Note that when F is a C^1-diffeomorphism between the open sets $U \subset R^n$ and $V \subset R^m$ then $n=m$ and DF(x) is nonsingular at all points $x \in U$.

A subset $M \subset R^n$ is a d-dimensional C^p-sub-manifold of R^n if for each point $x \in M$ there exists an open set $U \subset R^n$ containing x such that the neighborhood $U \cap M$ of x on M is C^p-diffeomorphic to an open subset V of R^d. Any particular diffeomorphism $F:U \cap M \to V$ is called a chart on $U \cap M$ and its inverse a local coordinate system on $U \cap M$.

Note that by this definition any open subset U of R^n is an n-dimensional C^∞-sub-manifold of R^n. The tangent space T_xU of this manifold U at any point $x \in U$ is the n-dimensional linear space $\{x\} \times R^n$ and the first and second tangent bundles TU and T^2U of U are the 2n- dimensional and 4n-dimensional submanifolds $U \times R^n$ of $(R^n)^2$ and $U \times (R^n)^3$ of $(R^n)^4$, respectively[3].

The classical example of a 2-dimensional C^∞-sub-manifold of R^3 is, of course, the unit sphere $S^2 = \{ (\xi,\eta,\zeta) \in R^3;\ \xi^2 + \eta^2 + \zeta^2 = 1 \}$. More generally,

[3]We use here the notation $(R^n)^k = R^n \times R^n \ldots \times R^n$ (k-times).

let $F: E \subset R^n \to R^m$, $n > m$, be some mapping of class C^ρ, $\rho \geq 1$, on the open set E of R^n. A point $x \in E$ is a regular point of F if dim $DF(x)R^n = m$; that is, if the derivative $DF(x)$ has full rank m. A point $b \in R^m$ is a regular value of F if the inverse image $F^{(-1)}(b) = \{ x \in E, F(x) = b\}$ consists only of regular points. Then the following result holds:

Theorem 1: Let $F: E \subset R^n \to R^m$, $n > m$, be a mapping of class C^ρ, $\rho \geq 1$, on the open set E of R^n. Then for any regular value $b \in R^m$ the inverse image $F^{(-1)}(b)$ is either empty or an (n-m)-dimensional C^ρ-sub-manifold of R^n.

From now on, let $F: E \subset R^n \to R^m$, $d = n - m > 0$, be a given mapping of class C^ρ, $\rho \geq 3$, on the non-empty open set E of R^n such that $DF(x)R^n = R^m$ for $x \in E$. Then each member of the family of sets

$$M_b = \{ x \in E, F(x) = b\}, \quad b \in F(E), \tag{2.1}$$

is a non- empty d-dimensional C^ρ-sub-manifold of R^n. Clearly, any point $x_0 \in E$ belongs to exactly one of these manifolds, namely that for $b = F(x_0)$; we shall call this the manifold of the family through the point x_0.

For any point $x \in M_b$ the tangent space $T_x M_b$ of M_b at x is defined by

$$T_x M_b = \{ (x,p) \in T_x R^n;\ DF(x)p = 0 \}. \tag{2.2}$$

Clearly, $T_x M_b$ is a d-dimensional linear subspace of the n-dimensional linear space $T_x R^n = \{x\} \times R^n$. The tangent bundle TM_b of M_b is the disjoint union of all tangent spaces $T_x M_b$ for $x \in M_b$; that is,

$$TM_b = \{ (x,p) \in TE;\ F(x) = b,\ DF(x)p = 0 \}. \tag{2.3}$$

In other words, the points $(x,p) \in TM_b$ are the zeroes of the mapping

$$H: E \times R^n \to R^m \times R^m;\ H(x,p) = \begin{pmatrix} F(x) - b \\ DF(x)p \end{pmatrix},\ \forall\, (x,p) \in E \times R^n$$

Since DF(x) was assumed to have full rank on E it follows that the derivative

$$DH(x,p) = \begin{pmatrix} DF(x) & 0 \\ D^2F(x)p & DF(x) \end{pmatrix}$$

has full rank on TE and hence, by Theorem 1, that the tangent bundle is a non-empty, 2d-dimensional $C^{\rho-1}$-sub-manifold of TR^n. Therefore, TM_b itself has a tangent bundle, namely, the 4d-dimensional $C^{\rho-2}$-sub-manifold $T(TM_b) = T^2M_b$ of the 4n-dimensional product space T^2R^n defined by

(2.4) $\quad T^2M_b = \{((x,y),(p,q)) \in T^2E;\ F(x)=b,\ DF(x)p = 0,\ DF(x)q+D^2F(x)(y,p)=0\}.$

3. <u>Vectorfields</u>

A C^σ-vectorfield, $\sigma \geq 1$, on some open subset E_0 of R^n is a C^σ-mapping on E_0 such that

(3.1) $\quad \pi\colon\ E_0 \to TE_0\,;\ \pi(x) = (x, \theta(x)),\ \forall\, x \in E_0\,.$

An integral curve of π through a point $x_0 \in E_0$ is any C^σ-path $\xi\colon J \to E_0$, defined on some open interval $J \subset R^1$ containing $0 \in J$, for which $(\xi(t),\xi'(t)) = \pi(\xi(t))$ for $t \in J$ and $\xi(0) = x_0$; that is, which solves the initial value problem

(3.2) $\quad x' = \theta(x),\ x \in E_0\,,\ x(0) = x_0.$

As before, let $F{:}E \subset R^n \to R^m$, $d=n-m > 0$, be a given mapping of class C^ρ, $\rho \geq 3$, on the non-empty open set E of R^n such that $DF(x)R^n = R^m$ for $x \in E$, and consider the family (2.1) of d-dimensional C^ρ-sub-manifolds of R^n. We call the vectorfield (3.1) tangential to this family of manifolds (2.1) if $\pi(x) \in T_xM_b$ for all $x \in E_0 \cap M_b$. Since $x \in M_b$, $b=F(x)$, for any $x \in E_0 \cap E$, this requires that

(3.3) $\quad DF(x)\theta(x) = 0,\ \forall\ x \in E_0 \cap E.$

Thus, for any integral curve $\xi: J \to E_0 \cap E$ of π through $x_0 \in E_0 \cap E$ it follows that $DF(\xi(t))\xi'(t) = 0$, $t \in J$. Since $\xi(J)$ is a connected subset of the open set $E_0 \cap E$, the integral mean-value theorem guarantees that

$$F(\xi(t)) - F(\xi(0)) = \int_0^t DF(\xi(s))\xi'(s)ds = 0, \ \forall\, t \in J.$$

In other words, the path $\xi: J \to E_0 \cap E$ remains on the manifold M_b, $b = F(x_0)$, through the initial point x_0, and (3.3) implies that $(\xi(t), \xi'(t)) \in TM_b$, for $t \in J$.

From this and the standard theory of ODEs (see e.g. [6] or [13]) we obtain now the following existence and uniqueness result:

Theorem 2: Let (3.1) be a C^σ-vectorfield, $\sigma \geq 1$, on the (non-empty) open subset E_0 of R^n. Then the following results hold:

(i) There exists a C^σ-integral curve $\xi: J \to E_0$ of π through each $x \in E_0$ defined on an open interval J containing 0. Moreover, any two such curves are equal on the intersection of their domains.

(ii) If π is tangential to the family (2.1) and $E_0 \cap E$ is non-empty, then any integral curve $\xi: J \to E_0 \cap E$ of π through $x_0 \in E_0 \cap E$ satisfies $(\xi(t), \xi'(t)) \in TM_b$, $b=F(x_0)$, for all $t \in J$.

(iii) The union of the domains of all integral curves of π through a point $x \in U_0$ is an open, possibly unbounded interval $J_x = (\tau_-(x), \tau_+(x))$. There exists a C^σ-integral curve $\xi^*: J_x \to E_0$, of π through x, and J_x is the largest interval on which such an intergal curve exists.

(iv) If $\tau_+(x) < \infty$ for some $x \in E_0$, then for any compact set $C \subset E_0$ there exists a $\delta > 0$ such that $\xi^*(t) \notin C$ for $t > \tau_+(x) - \delta$. A corresponding result holds when $\tau_-(x) > -\infty$.

(v) The set $D(\pi) = \{(t,x) \in R^1 \times U_0;\ t \in J_x\}$ is open in $R^1 \times E_0$ and contains $\{0\} \times U_0$. Moreover, the global flow $\gamma: D(\pi) \to E_0$, $\gamma(t,x) = \xi^*(t)$, $t \in J_x$, of π is of class C^σ on $D(\pi)$.

Consider now a second order initial value problem $x'' = \theta(x,x')$, $x \in E_0$,

$x(0)=x_0$, $x'(0)=y_0$, which, of course, may be written in the first order form

(3.4) $$x' = y,\ \ y' = \theta(x,y),\ x \in E_0,\ x(0) = x_0,\ x'(0) = y_0.$$

Thus, we encounter in this case a vector-field of the form

(3.5) $$\pi\colon E_\pi = E_0 \times Y \subset TE_0 \to T^2E_0\ ;\ \pi(x,y) = ((x,y),(y,\theta(x,y))),\ \ \forall\ (x,y) \in E_0 \times Y$$

on a subset of the tangent bundle TE_0 of E_0. Note that the second and third component of the image vector are identical. In other words, (3.5) represents a sub-class of the vector fields on E_π called the vector fields on E_π that are consistent with a second order ODE. We assume always that the domain E_π of π is some open subset of TE_0.

An integral curve of (3.5) through a point $(x_0, y_0) \in E_\pi$ is now a C^σ-path $\xi\colon J \to E_0$, defined on some open interval $J \subset R^1$ containing $0 \in J$, for which

(3.6) $$\begin{aligned} &(\xi(t),\ \xi'(t)) \in E_\pi\ ,\ \xi(0)=x_0,\ \xi'(0)=y_0 \\ &((\xi(t),\xi'(t)),(\xi'(t),\xi''(t))) = \pi(\xi(t),\xi'(t)),\ \forall\ t \in J; \end{aligned}$$

that is, which is a solution of the initial value problem (3.4).

As before, the vectorfield (3.5) is called tangential to the family of tangent bundles TM_b, $b \in F(E)$, of (2.1) if $\pi(x,y) \in T_{(x,y)}(TM_b)$ for $(x,y) \in E_\pi \cap TM_b$; that is, if

(3.7) $$DF(x)\theta(x,y) + D^2F(x)(y,y) = 0,\ \forall\ (x,y) \in E_\pi \cap (E \times \ker DF(x))$$

Then, for any integral curve $\xi\colon J \to E_0 \cap E$, of π through $(x_0,y_0) \in E_\pi \cap TM_b$ such that $DF(\xi(t))\xi'(t) = 0$, $t \in J$, the integral mean-value theorem provides that

$$DF(\xi(t))\xi'(t) - DF(x_0)y_0 = \int_0^t [DF(\xi(s))\xi''(s) + D^2F(\xi(s))(\xi'(s),\xi'(s))]ds = 0,\ \ \forall\ t \in J$$

Hence, the path $\xi:J \to E_0 \cap E$ remains on the tangent bundle TM_b, $b = F(x_0)$, corresponding to x_0 and (3.7) implies that $((\xi(t),\xi'(t)),(\xi'(t),\xi''(t))) \in T^2M_b$, for $t \in J$.

Again an existence and uniqueness result of the form of Theorem 2 holds. We note here only the following shortened version.

Theorem 3: Let (3.5) be a C^σ-vectorfield, $\sigma \geq 2$, on the (non-empty) open subset $E_\pi \subset TE_0 \subset TR^n$. Then there exists an integral curve $\xi: J \to U_0$ of π through each $(x,y) \in E_\pi$ defined on an open interval J containing 0. Moreover, any two such curves are equal on the intersection of their domains. If π is tangential to the family (2.1) and $E_0 \cap E$ is non-empty, then any integral curve $\xi:J \to E_0 \cap E$ of π through $(x_0,y_0) \in E_\pi \cap TM_b$, $b=F(x_0)$, for which $DF(\xi(t))\xi'(t) = 0$ for t in J, satisfies $((\xi(t),\xi'(t)),(\xi'(t),\xi''(t))) \in T^2M_b$, for all $t \in J$.

4. A Class of First and Second Order DAEs

In this section we begin with the autonomous, first order DAE

$$\begin{aligned} F_1(x) &= b \\ F_2(x, x', z) &= 0 \end{aligned} \tag{4.1}$$

for which we assume that

(4.2a) $F_1: E_x \subset R^n \to R^r$ and $F_2: E_2 = E_x \times E_p \times E_z \subset (R^n)^2 \times R^m \to R^s$ are of class C^ρ, $\rho \geq 3$, on their domains, where $E_x \subset R^n$, $E_p \subset R^n$, and $E_z \subset R^m$, are non-empty open sets, and $r<n\leq r+s=n+m$; and

(4.2b) for each $(x,p,z) \in E_2$ the matrix

$$\begin{pmatrix} DF_1(x) & 0 \\ D_pF_2(x,p,z) & D_zF_2(x,p,z) \end{pmatrix}$$

is non-singular.

From (4.2b) it follows that $DF_1(x)R^n = R^r$ for all $x \in E_x$ and hence, as we saw in section 2, that each member of the family of sets

(4.3) $$M_b = \{ x \in E_x, F_1(x) = b\},\ b \in F_1(E_x),$$

is a non- empty (n-r)-dimensional C^ρ-sub-manifold of R^n. For any $x_0 \in E_x$ we call the unique manifold (4.3) with $b = F_1(x_0)$ the constraint manifold through that point.

For given $b \in F_1(E_x)$ a C^σ-solution, $1 \le \sigma \le \rho-1$, of (4.1) consists of two C^σ-paths $x: J \to E_x$ and $z: J \to E_z$, defined on some open interval J of R^1, such that

(4..4) $$(x(t),x'(t),z(t)) \in E_2\ ,\ F_1(x(t)) = b,\ F_2(x(t),x'(t),z(t)) = 0,\ \forall t \in J.$$

This necessitates that $DF_1(x(t))x'(t) = 0$, $\forall t \in J$. Hence, if $(x_0,p_0,z_0) \in E_2$ is any point on a solution (4.4); that is, if $x(t_0) = x_0$, $x'(t_0) = p_0$, $z(t_0) = z_0$ for some $t_0 \in J$, then we must have $DF_1(x_0)p_0 = 0$, and $F_2(x_0,p_0,z_0) = 0$, while, of course, automatically $x_0 \in M_b$ for $b=F_1(x_0)$.

This suggests the definition of the <u>initial data map</u>

(4.5) $$H: E_2 \to R^r \times R^s,\ H(x,p,z) = \begin{pmatrix} DF_1(x)p \\ F_2(x,p,z) \end{pmatrix},\ (x,p,z) \in E_2\,.$$

Evidently, for any given $(x,p,z) \in E_2$, the partial derivative $D_{p,z}H$ of H with respect to p and z is the matrix in (4.2b). By Theorem 1 this implies that

(4.6) $$K = \{ (x,p,z) \in E_2\ ;\ H(x,p,z) = 0 \}$$

is a n-dimensional $C^{\rho-1}$-submanifold of $(R^n)^2 \times R^m$, the <u>initial data manifold</u> of the problem.

A general existence and uniqueness theory for (4.1) was given in [12] and requires a closer analysis of the relationship between the initial data manifold K and the constraint manifolds (4.3) utilizing the theory of covering spaces. For the applications considered here it suffices to restrict attention to the case when F_2 is linear in p and z; that is, when (4.1) has the special form

$$(4.7)\qquad \begin{aligned} F_1(x) &= b \\ A(x)x' + B(x)z + G(x) &= 0, \end{aligned}$$

Here (4.2a) requires that F_1: $E_x \subset R^n \to R^r$, $A: E_x \to L(R^n,R^s)$, $B: E_x \to L(R^n,R^s)$, and $G: E_x \to R^s$ are of class C^ρ, $\rho \geq 3$, on the open non-empty set $E_x \subset R^n$, and that $r<n \leq r+s=n+m$. Moreover, condition (4.2b) is equivalent with the assumption that for each $x \in E_x$ the matrix

$$(4.8)\qquad \begin{pmatrix} DF_1(x) & 0 \\ A(x) & B(x) \end{pmatrix}$$

is non-singular.

Hence, in this case the equation $H(x,p,z) = 0$ has for each $x \in E_x$ a unique solution

$$(4.9)\qquad \begin{pmatrix} p \\ z \end{pmatrix} = \begin{pmatrix} \eta(x) \\ \zeta(x) \end{pmatrix} = \begin{pmatrix} D_1F(x) & 0 \\ A(x) & B(x) \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ -G(x) \end{pmatrix}$$

Then

$$(4.10)\qquad \pi: E_x \to TE_x, \quad \pi(x) = (x, \eta(x)), \quad x \in E_x$$

defines a C^ρ-vectorfield on the open set E_x which by definition of the initial data manifold K is tangential to the family of constraint manifolds (4.3). Now, consider (4.7) together with the initial condition $x(0) = x_0 \in E_x$ and set $p_0=\eta(x_0)$, $z_0=\zeta(x_0)$ which implies that $(x_0, p_0, z_0) \in K$. Then Theorem 3 holds and there exists an integral curve $\xi: J \to E_x$ of π through x_0 for which $(\xi(t),\xi'(t)) \in TM_b$, $b=F(x_0)$, for all $t \in J$. In other words, the paths $x: J \to E_x$, $z: J \to E_z$, defined by $x(t)=\xi(t)$, $z(t)=\zeta(\xi(t))$, $t \in J$, constitute a solution of (4.7).

Instead of repeating all of Theorem 3 we summarize this result only as follows:

Theorem 5: If (4.2a/b) holds for (4.7), then, for any given $x_0 \in E_x$, there exists a unique, maximally extended C^r-solution $x: J \to E_1$ and $z: J \to E_z$, of (4.7) which satisfies the initial conditions $x(0) = x_0$, $x'(0) = p_0 = \eta(x_0)$, $z(0) = z_0 = \zeta(x_0)$.

As noted, a corresponding result for the general equation (4.1) was proved in [12]. There the theory was also extended to the second order system

$$\begin{aligned} F_1(x) &= b \\ F_2(x, x', x'', z) &= 0 \end{aligned} \tag{4.11}$$

subject to the conditions

(4.12a) $F_1: E_x \subset R^n \to R^r$ and $F_2: E_2 = E_x \times E_y \times E_q \times E_z \subset (R^n)^3 \times R^m \to R^s$ are of class C^ρ, $\rho \geq 4$, on their domains where $E_x, E_y, E_z \subset R^n$, and $E_z \subset R^m$, are non-empty open sets and $r < n \leq r+s = n+m$;

(4.12b) for each $(x,y,q,z) \in E_2$ the matrix

$$\begin{pmatrix} DF_1(x) & 0 \\ D_qF_2(x,y,q,z) & D_zF_2(x,y,q,z) \end{pmatrix}$$

is non-singular.

As before we see that each member of the family of sets (4.3) is a non-empty (n-r)-dimensional C^ρ-sub-manifold of R^n, the constraint manifold of (4.11) through x_0.

It is natural to reduce (4.11) to the first order system:

$$\begin{aligned} F_1(x) &= b \\ x' - y &= 0 \\ F_2(x, y, y', z) &= 0. \end{aligned} \tag{4.13}$$

With the combination (x,y) as new differential variable, this constitutes a DAE of the form (4.1) for which (4.2a) turns out to be valid. However, (4.2b) does not hold since the corresponding matrix

$$\begin{pmatrix} DF_1(x) & 0 & 0 \\ I_n & 0 & 0 \\ 0 & D_qF_2(x,y,q,z) & D_zF_2(x,y,q,z) \end{pmatrix}$$

is singular. This failure of (4.2b) is hardly surprising since we should expect (4.11) to induce a vector field on the tangent bundle TE_x that is consistent with a second order equation.

For any $b \in F_1(E_x)$ a C^σ-solution, $1 \le \sigma \le \rho-2$, of (4.1) consists of C^σ- paths $x: J \to E_x$ and $z: J \to E_z$, defined on some open interval J of R^1, such that

(4.14) $\quad (x(t),x'(t),x''(t),z(t)) \in E_2,\ F_1(x(t)) = b,\ F_2(x(t),x'(t),x''(t),z(t)) = 0,\ \forall\, t \in J.$

This implies that $DF_1(x(t))x'(t) = 0$, $DF_1(x(t))x''(t) + D^2F_1(x)(x'(t),x'(t))=0$, for all t in J, which means that $\gamma: J \to T^2M_b$, $\gamma(t) = ((x(t),x'(t)),(x'(t),x''(t)),\ t \in J$, is a path on T^2M_b. In analogy to the first order case, this suggests the definition

(4.15) $\quad H: E_2 \subset (R^n)^3 \times R^m \to R^{r+s}$

$$H(x,y,q,z) = (DF_1(x)q + D^2F_1(x)(y,y),\ F_2(x,y,q,z))\ ,\ \forall\ (x,y,q,z) \in E_2$$

for the initial data map of (4.11). Once again, (4.12b) implies that the solution set

(4.16) $\quad K = \{ (x,y,q,z) \in E_2\ ;\ H(x,y,q,z) = 0 \}$

is an n-dimensional $C^{\rho-2}$-submanifold of $(R^n)^3 \times R^m$, called the initial data manifold of (4.11).

As before, we shall not present here the general theory but restrict ourselves to the linear case

(4.17)
$$\begin{aligned} F_1(x) &= b \\ A(x,x')x'' + B(x,x')z + G(x,x') &= 0, \end{aligned}$$

Then (4.12a) requires that the maps $F_1: E_x \subset R^n \to R^r$, $A: E_x \times E_y \to L(R^n,R^s)$, $B: E_x \times E_y \to L(R^m,R^s)$ and $G: E_x \times E_y \to R^s$ are of class C^ρ, $\rho \geq 4$, on their domains where $E_x, E_y \subset R^n$ are non-empty open sets and $r<n\leq r+s=n+m$. Moreover, (4.12b) is equivalent with the assumption that the matrix

$$(4.18) \qquad \begin{pmatrix} DF_1(x) & 0 \\ A(x,y) & B(x,y) \end{pmatrix}$$

is non-singular for all $(x,y) \in E_x \times E_y$.

Then, as in the first order case, the equation $H(x,y,q,z) = 0$ has for each (x,y) in $E_x \times E_y$ a unique solution

$$(4.19) \qquad \begin{pmatrix} q \\ z \end{pmatrix} = \begin{pmatrix} \eta(x,y) \\ \zeta(x,y) \end{pmatrix} \equiv -\begin{pmatrix} DF_1(x) & 0 \\ A(x,y) & B(x,y) \end{pmatrix}^{-1} \begin{pmatrix} D^2F_1(x)(y,y) \\ G(x,y) \end{pmatrix}$$

and hence

$$(4.20) \qquad \pi: E_\pi = E_x \times E_y \subset TE_x \to T^2E_1, \quad \pi(x) = ((x,y),(y,\eta(x,y))), \quad (x,y) \in E_\pi$$

defines a $C^{\rho-1}$-vectorfield on the open set E_π of the tangent bundle TE_x. Clearly, by definition of the initial data manifold K, this vectorfield is tangential to the family of tangent bundles TM_b, $b \in F_1(E_x)$ of the constraint manifolds (4.3) of (4.17); that is,

$$(4.21) \qquad DF_1(x)\eta(x,y) + D^2F_1(x)(y,y) = 0, \ \forall\ (x,y) \in E_x \times (E_y \cap \ker DF_1(x))$$

Now, consider (4.17) together with the initial condition

$$(4.22) \qquad x(0) = x_0\ ,\ y(0) = y_0\ ,\ (x_0,y_0) \in E_x \times (E_y \cap \ker DF_1(x_0))$$

and set $q_0=\eta(x_0,y_0)$, $z_0=\zeta(x_0,y_0)$ which implies that $(x_0,y_0,q_0,z_0) \in K$. Thus by Theorem 3 there exists an integral curve $\xi: J \to E_x$ of π for which (3.6) holds. By definition of π we have $((\xi(t),\xi'(t)),(\xi'(t),\xi''(t))) \in K$, $t \in J$, and hence, in particular $DF_1(\xi(t))\xi'(t) = 0$, $t \in J$. Thus it follows that $((\xi(t),\xi'(t)),(\xi'(t),\xi''(t))) \in$

T^2M_b, $b=F_1(x_0)$, and therefore that the paths $x:J \to E_x$, $z:J \to E_z$, defined by $x(t)=\xi(t)$, $z(t)=\zeta(\xi(t))$, $t \in J$, constitute a solution of (4.7).

Once again, instead of repeating all of Theorem 4 we summarize this result only in the brief form:

Theorem 6: If (4.12a/b) holds for (4.17), then, for any given initial data (4.22), there exists a unique, maximally extended C^p-solution $x: J \to E_x$, $z: J \to E_z$, of (4.17) which satisfies the initial conditions $x(0) = x_0$, $x'(0) = y_0$, $x''(0)=\eta(x_0,y_0)$, $z(0) = \zeta(x_0,y_0)$.

For a corresponding result for the general equations (4.11) see again [12].

5. Local Parametrizations

As shown in [12] the results about the semi-implicit DAEs (4.1) and (4.11) lead to a general local parametrization approach for the numerical solution of these systems. Once again, we shall restrict our discussion here to the linear systems (4.7) and (4.17).

Consider first the system (4.7), and suppose that we are in the setting of Theorem 5. Thus, we wish to compute a numerical approximation of the unique C^p-solution $x: J \to E_x$, $z: J \to E_z$ of (4.7) which satisfies the initial conditions $x(0) = x_0$, $p_0 = \eta(x_0)$, $z_0 = \zeta(x_0)$ for given $x_0 \in E_x$. Here $\eta:E_x \to E_p$ and $\zeta:E_x \to E_z$ are the mappings (4.9). As we saw, the problem of solving (4.7) in E_x then reduces to that of solving the explicit initial value problem

(5.1) $$x'= \eta(x),\ x \in E_x,\ x(0) = x_0.$$

Since the desired solution $x: J \to E_0$ of (5.1) through x_0 remains on the tangent bundle TM_b of the constraint manifold M_b, $b =F(x_0)$, through x_0 it is natural to work with a local coordinate system on M_b.

Consider any point $x_c \in M_b$, on the manifold M_b through x_0. The subscript 'c' indicates here that x_c will later represent a 'current' (approximate) point on the solution. Now choose a linear subspace $T \subset R^n$, dim $T = n\text{-}r$, such that $T^\perp \cap \ker D_1F(x_c) = \{0\}$. Then it follows from the implicit function theorem that there exist open neighborhoods V of the origin in T and S_x of x_c in R^n, respectively, as well as a C^p-map $w: V \to T^\perp \subset R^n$ with $w(0) = 0$, such that $M_b \cap S_x = \Psi(V)$ where Ψ is the local coordinate map

$$(5.2) \qquad \Psi: V \to R^n, \ \Psi(t) = x_c + t + w(t), \ t \in V.$$

In practice it is often useful to work with local coordinate mappings that correspond to the tangent spaces of M_b; that is, to choose $T = \ker DF(x_c)$. Note that then $Dw(0) = 0$, (see, e.g., [11]).

For the computation we introduce orthonomal bases

$$(5.3) \qquad \begin{aligned} &Q_1 \in L(R^{n-r}, R^n), \ Q_2 \in L(R^r, R^n), \\ &Q_1 R^{n-r} = T, \ Q_2 R^r = T^\perp \\ &Q_1^* Q_1 = I_{n-r}, \ Q_2^* Q_2 = I_r, \ Q_2^* Q_1 = 0 \end{aligned}$$

for T and $T^\perp$. Then we have the transformed local coordinate map

$$(5.4) \qquad \Phi: U = Q_1^{-1} V \to R^n, \ \Phi(u) = x_c + Q_1 u + Q_2 \omega(u), \ u \in U \subset R^{n-r}$$

where $\omega(u) = (Q_2|T^\perp)^{-1} w((Q_1|T)^{-1} u)$, $u \in U$, is again of class C^p and satisfies $\omega(0)=0$. From $F_1(\Phi(u)) = 0$ we find that $D\Phi(u)R^{n-r} \subset \ker DF_1(\Phi(u))$ for $u \in U$ and, by (5.3), that

$$(5.5) \qquad Q_1^* D\Phi(u) = Q_1^*[Q_1 + Q_2 D\omega(u)] = I_{n-r}$$

whence, by a dimensionality argument,

$$(5.6) \qquad D\Phi(u)R^{n-r} = \ker DF_1(\Phi(u)), \ \forall\, u \in U.$$

This implies that for any $u \in U$ and $c \in \ker DF_1(\Phi(u))$ the equation $D\Phi(u)a=c$

has a solution $a \in R^{n-r}$ for which $a = Q_1^* c$ and hence which is unique.

In our local coordinate system we obtain for the ODE (5.1) the local representation

(5.7a) $$D\Phi(u)u' = \eta(\Phi(u)),\ u \in U$$

which, because of $\eta(\Phi(u)) \in \ker DF_1(\Phi(u))$, can be written in the form of the (n-r)-dimensional explicit system

(5.7b) $$u' = Q_1^*\, \eta(\Phi(u)),\ u \in U.$$

Obviously, with $p = Q_1\eta_1 + Q_2\eta_2$, $\eta_1 \in R^{n-r}$, $\eta_2 \in R^r$, the equation $H(x,p,z) = 0$ becomes the non-singular, linear system

(5.8) $$\begin{pmatrix} DF_1(x)Q_1 & DF_1(x)Q_2 & 0 \\ A(x)Q_1 & A(x)Q_2 & B(x) \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ G(x) \end{pmatrix}$$

Hence, if, for given $x = \Phi(u)$, $u \in U$, the solution of (5.8) has been found then we have $Q_1^*\, \eta(\Phi(u)) = \eta_1$ and $\zeta(\Phi(u)) = z$.

This local parametrization can also be carried over to the second order system (4.17). As before, suppose that we are in the setting of Theorem 6. Thus, we wish to compute a numerical approximation of the unique C^{p-1}-solution $x: J \to E_x$, $z: J \to E_z$ of (4.17) which satisfies the initial conditions $x(0)=x_0$, $x'(0)=y_0$, $x''(0)=\eta(x_0,y_0)$, $z(0)=\zeta(x_0,y_0)$ where $(x_0,y_0) \in E_x \times E_y \cap TM_b$, $b=F_1(x_0)$, are given and $\eta: E_\pi = E_x \times E_y \to E_q$, $\zeta: E_x \times E_y \to E_z$, are the mappings (4.19). As we saw, the problem of solving (4.17) reduces to that of solving the explicit system

(5.9) $$x' = y,\ y' = \eta(x,y),\quad (x,y) \in E_\pi,\ x(0)=x_0,\ y(0)=y_0,$$

Since the desired solution $x: J \to E_x$ of (5.1) through x_0 remains on the second tangent bundle T^2M_b of the constraint manifold M_b through x_0 we are led to working with a local coordinate system on TM_b.

Once again let x_c be a 'current' point on the manifold M_b through x_0 and choose a linear subspace $T \subset R^n$, dim $T = n-r$, such that $T^{\perp} \cap \ker DF(x_0) = \{0\}$. Then, with basis maps Q_1, Q_2 satisfying (5.3), the local coordinate map (5.4) is well defined and

$$(5.10) \qquad \Theta : U \times R^{n-r} \to TM_b,\ \Theta(u,v) = (\Phi(u), D\Phi(u)v),\ \ u \in U,\ v \in R^{n-r}$$

defines a local coordinate system on TM_b. Clearly, we can choose some neighborhood S_0 of the origin of $U \times R^{n-r}$ such that $\Theta(u,v)$ belongs to E_π for all (u,v) in S_0.

Thus with $x = \Phi(u)$ and $y = D\Phi(u)v = Q_1v + Q_2D\omega(u)v$, the differential equations (5.9) assume the local form

$$(5.11) \qquad \begin{aligned} &D\Phi(u)u' = Q_1v + Q_2D\omega(u)v \\ &D\Phi(u)v' + D^2\Phi(u)(u',v) = \eta(\Phi(u), Q_1v + Q_2D\omega(u)v). \end{aligned}$$

Recall that for any $d \in \ker DF_1(\Phi(u))$ the unique solution of $D\Phi(u)a = d$ is $a = Q_1^*d$. Hence, since $Q_1v + Q_2D\omega(u)v \in \ker DF_1(x)$, the first equation reduces simply to $u' = v$ and, with this, the second equation can be written as

$$D\Phi(u)v' = \eta(x,y) - D^2\Phi(u)(v,v)\ ,\ x = \Phi(u),\ y = Q_1v + Q_2D\omega(u)v.$$

From $DF_1(\Phi(u))D\Phi(u) = 0$, it follows, together with (4.21) and (5.9), that

$$(5.12) \qquad \begin{aligned} 0 &= DF_1(x)D^2\Phi(u)(v,v) + D^2F_1(x)(D\Phi(u)v, D\Phi(u)v) \\ &= DF_1(x)D^2\Phi(u)(v,v) + D^2F_1(x)(y,y) \\ &= DF_1(x)[D^2\Phi(u)(v,v) - \eta(x,y)] \quad ,\ \forall\ (u,v) \in S_0 \end{aligned}$$

and, therefore that, as desired, $\eta(x,y) - D^2\Phi(u)(v,v) \in \ker DF_1(x)$.

With this we have shown now that on S_0 the equations (5.11) can be reduced to the explicit form

$$(5.13)\qquad \begin{aligned} u' &= v \\ v' &= Q_1^* \left[\eta(\Phi(u), Q_1 v + Q_2 D\omega(u)v) - D^2\Phi(u)(v,v)\right]. \end{aligned}$$

From (5.5) it follows that $Q_1^* D^2\Phi(u)=0$, so that (5.13) reduces to

$$(5.14)\qquad \begin{aligned} u' &= v \\ v' &= Q_1^*\eta(\Phi(u), Q_1 v + Q_2 D\omega(u)v) = Q_1^*\eta(\Phi(u), D\Phi(u)v) \end{aligned}$$

Now , with $\eta(x,y)=Q_1\eta_1 + Q_2\eta_2$, $\eta_1 \in R^{n-r}$, $\eta_2 \in R^r$, the equation $H(x,y,q,z) = 0$ becomes the non-singular, linear system

$$(5.15)\qquad \begin{pmatrix} DF_1(x)Q_1 & DF_1(x)Q_2 & 0 \\ A(x,y)Q_1 & A(x,y)Q_2 & B(x,y) \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \\ z \end{pmatrix} = -\begin{pmatrix} D^2F_1(x)(y,y) \\ G(x,y) \end{pmatrix}$$

Hence, if, for given $x = \Phi(u)$, $y = D\Phi(u)v$, $(u,v) \in S_0$, a solution of (5.15) has been obtained then $v' = Q_1^*\eta(\Phi(u),D\Phi(u)v) = \eta_1$ and $z = \zeta(\Phi(u),D\Phi(u)v)$.

6. Computational Implementation of the Local Parametrization

In the previous section we have used the local coordinate map (5.4) to reduce the semi-implicit DAEs (4.7) and (4.17) to the explicit systems of ODEs (5.7b) and (5.14), respectively. Theoretically any ODE solver can be applied to these ODE systems to obtain a local solution of the original DAE. Before discussing this in more detail, we consider first how the local coordinate map Φ of (5.4) at the current point x_c of the constraint manifold M_b, $b = F_1(x_0)$, may be implemented and how we might choose the matrices Q_1 and Q_2 that define this local parametrization.

By definition, for any given $u \in U$, the point $x = \Phi(u)$ on M_b is the solution of the augmented system

$$(6.1)\qquad \begin{pmatrix} F_1(x) \\ Q_1^*(x - x_c) \end{pmatrix} = \begin{pmatrix} b \\ u \end{pmatrix}$$

Here, of course, the matrices Q_1, Q_2 are assumed to satisfy (5.3) and the subspace $T=Q_1^*R^{n-r}$ has to induce a local parametrization of M_b at x_c; that is, we have

$$(6.2) \qquad (Q_1^* R^{n-r})^{\perp} \cap \ker DF_1(x_c) = \{0\}.$$

It is readily seen that (6.2) holds if and only if the Jacobian

$$(6.3) \qquad \begin{pmatrix} DF_1(x) \\ Q_1^* \end{pmatrix}$$

of the mapping on the left side of (6.1) is nonsingular at x_c which, in turn is equivalent with the nonsingularity of $DF_1(x_c)Q_2$.

As proved, for instance, in [7], under this nonsingularity assumption there exists an open set $U_1 \subset U$ containing the origin, such that for any u in U_1 Newton's method applied to (6.1) and started from $y^{(0)} = x_c + Q_1u$ produces a sequence of points $\{y^{(k)}\}$ that converges Q-quadratically to $x=\Phi(u)$. A step of this process here has the algorithmic form:

(1) Evaluate $a_1 = F_1(y^{(k)}) - b$, $a_2 = Q_1^*(y^{(k)} - x_c)$;
(2) solve the linear system

$$\begin{pmatrix} DF_1(y^{(k)}) \\ Q_1^* \end{pmatrix} s = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix};$$

(3) set $y^{(k+1)} = y^{(k)} - s$.

Observe that for our choice $y^{(0)} = x_c + Q_1u$ of the starting point the iterates $y^{(k)}$ remain in the affine subspace $x_c + Q_2R^r$.

Let $s_1 = Q_1^*s$, $s_2 = Q_2^*s$, then, by (5.3), we have $s = Q_1s_1 + Q_2s_2$ and we obtain the solution of the linear system in step (2) by setting $s_1=a_2$ and solving the (n-r)-dimensional linear system

(6.4) $$[DF_1(y^{(k)})Q_2]\, s_2 = a_1 - DF_1(x^{(k)})\, Q_1 a_2 .$$

Thus, when the Jacobian of $F_1(x)$ is readily available, then Newton's method provides an efficient numerical procedure for implementing the local coordinate map (5.4).

We turn now to the construction of the matrices Q_1, Q_2 for which (5.3) and (6.2) are satisfied . Two choices appear to be particularly useful in practice. The first one was already mentioned in the previous section and defines the parametrization by using the space $T = \ker DF_1(x_c)$ corresponding to the tangent space of M_b at x_c. In this case the matrices Q_1, Q_2 may be obtained, for instance, by performing a QR-factorization of the transposed Jacobian of F_1

(6.5) $$DF_1(x_0)^* = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$$

where Q is an nxn unitary matrix and R an rxr upper triangular matrix which, by (4.2b) is non-singular. In fact, it follows easily that then the local parametrization is defined by the matrices

(6.6) $$Q_2 = Q(e_1, \ldots, e_r)\, , \; Q_1 = Q(e_{r+1}\, , \ldots , e_n)$$

formed from the first r and last n-r columns of Q, respectively. Here $e_1, \ldots, e_n$ denote the natural basis vectors of R^n.

This "tangent space" parametrization may be somewhat costly to use. To reduce the cost it is advantageous to choose a local coordinate space T which is spanned by n-r suitably selected natural basis vectors of R^n. If, say,

(6.7) $$T^{\perp} = \text{span}\,\{ e_{j_1}, \ldots, e_{j_r} \},\; T = \text{span}\,\{ e_{j_{r+1}}, \ldots, e_{j_n} \}$$

then the condition $T^{\perp} \cap \ker DF(x_c) = \{0\}$ requires that we select the indices $j_1, \ldots, j_r$ such that the corresponding columns of $DF(x_c)$ are linearly independent. It is well-known that such a choice may be derived, for instance, from a Jordan factorization with row and column pivoting, or from a singular value decomposition (SVD) of $DF_1(x_c)$ (see.e.g. [3]). The matrices of the local parametrization induced by (6.6) then are

$$(6.8) \qquad Q_1 = (e_{j_{r+1}}, ..., e_{j_n}), \quad Q_2 = (e_{j_1}, ..., e_{j_r})$$

and satisfy (5.3) by construction.

The choice of the permutation $[j_1,...,j_n]$ in (6.7) and (6.8) "partitions" the components of any vector x into a vector $\xi_1 = Q_1x$ of " independent coordinates " and a vector $\xi_2 = Q_2x$ of "dependent coordinates ". Thus it is natural to call (6.8) a local parametrization by "coordinate partitioning".

7. Explicit and Implicit Multistep Methods

Consider again the first-order DAE (4.7) under the assumptions (4.2a/b) which, by Theorem 5, guarantee the existence of a solution $x:J \to E_x$, $z:J \to E_z$ that satisfies the initial conditions $x(0) = x_0$, $x'(0) = p_0 = \eta(x_0)$, $z(0) = z_0=\zeta(x_0)$ corresponding to the given point $x_0 \in M_b$ on the constraint manifold.

Suppose that $x_c = x(t_c) \in M_b$ is a 'current' point on this solution where a local parametrization (5.4) has been constructed. In some region near x_c we wish to compute a sequence of approximation

$$(7.1) \qquad x_i \cong x(t_i),\ z_j \cong z(t_i),\ t_i= t_c+ ih\ ,\ i=1,2,...,N$$

of points $x(t_k)$ along the solution. More precisely, we suppose that the constants h and N are chosen such that the points $x(t_k)$ belong to the neighborhood of x_c where the local parametrization (5.4) is valid Then, if u is the solution of (5.7b) satisfying the initial condition $u(t_c)=0$, it follows that

$$(7.2) \qquad x(t_k) = \Phi(u(t_k)) \quad k=1,2,...,N,\ x(t_c) = \Phi(u(t_c)) = x_c.$$

For the approximate solution of (5.7b) we consider a multistep method of the general form

$$u_k = \sum_{i=1}^{p} \alpha_i u_{k-i} + \sum_{i=0}^{p} \beta_i u'_{k-i}\,, \quad u'_{k-i} = Q_1^* \eta(\Phi(u_{k-i})) \tag{7.3}$$

which is assumed to be consistent; that is,

$$\sum_{i=1}^{p} \alpha_i = 1, \tag{7.4}$$

as well as convergent of order $\upsilon \geq 1$. Assume that for some k, $1 \leq k \leq N$, the approximations

$$u_j \cong u(t_j)\,,\ x_j \cong \Phi(u_j)\,,\ j=0,1,\ldots k-1, \tag{7.5}$$

have already been computed. Then the next point $u_k \cong u(t_k)$ along the solution of (5.7b) is specified by (7.3) and, by solving the equation (6.1) with $u = u_k$, we obtain $x_k = \Phi(u_k)$ as the next approximation of the solution of (4.7).

As shown in section 5, the vectors u'_{k-i} of (7.3) are the solutions of a linear system of the form (5.8). We consider first the case $\beta_0 = 0$ of explicit integration. Since the local coordinate map (5.4) is defined by the matrices Q_1, Q_2 we have, by (6.1),

$$u = Q_1^*(x-x_c) \quad . \tag{7.6}$$

In other words, we may assume that the computed approximations (7.4) satisfy

$$u_j = Q_1^*(x_j-x_c), \quad j = 1,2,\ldots,k-1 \quad . \tag{7.7}$$

Together with (7.6) this implies that when u_k is determined by the multistep method (7.3) then, instead of using (6.1) with $u = u_k$, we may obtain $x_k= \Phi(u_k)$ as a solution of the nonlinear system

$$(7.8)\qquad \begin{pmatrix} F_1(x) - b \\ Q_1^* x - \sum_{i=1}^{p} [\alpha_i x_{k-i} + h\beta_i \eta(x_{k-i})] \end{pmatrix} = 0$$

This leads to the following algorithm for computing from the last p known approximations

$$(7.9)\qquad x_{k-j} \equiv x(t_{k-j}),\ z_{k-j} \equiv z(t_{k-j}),\ w_{k-j} \equiv \eta(x_{k-j}),\ j = 1,2,\dots,p$$

a next approximate point on the desired solution of (4.7):

<u>Algorithm 1.</u> (1) Evaluate $a_k = Q_1^*(\sum_{i=1}^{p} \alpha_i x_{k-i} + h\sum_{i=1}^{p} \beta_i w_{k-i})$

(2) Compute the solution x_k of the nonlinear system

$$\begin{pmatrix} F_1(x) - b \\ Q_1^* x - a_k \end{pmatrix} = 0$$

(3) With $x = x_k$ solve the linear system (5.8) to obtain $w_k = Q_1\eta_1$ and $z_k = z$.

This algorithm may be applied as long as the computed points do not leave the region of validity of the local parametrization at x_c defined by Q_1 and Q_2. To determine when the points leave this region is a very delicate problem and requires special attention. In our numerical implementation we decide to change the local parametrization when the estimated condition number of the Jacobian of the system in step (2) becomes too large or when the number of Newton steps required for solving this system exceeds a certain bound . Of course, if the multistep method (7.3) has order υ then one should solve the systems in step (2) and (3) with an error not exceeding $O(h^{\upsilon+1})$.

A further delicate problem is the initialization of the overall process. One approach is to obtain $u_1, u_2, \ldots, u_p$ by means of some known start-up process for the multistep method (7.3) applied to the ODE (5.7b) and then to set

$$x_i = \Phi(u_i)\,,\quad w_i = \eta(x_i)\,,\ i = 1,2,\ldots,p$$

by solving the corresponding systems (6.1) and (5.8) . Numerical experience indicates that no reinitialization is necessary when passing from one local parametrization to another.

In the case $\beta_0 \neq 0$ the new point is implicitely defined by both (7.3) and (5.8); that is, the systems in step (2) and (3) of algorithm 1 can no longer be solved separately. Thus, in this case the algorithm has to be modified as follows:

Algorithm 2. (1) Evaluate $a_k = Q_1^*\left(\sum_{i=1}^{p} \alpha_i x_{k-i} + h\sum_{i=1}^{p} \beta_i w_{k-i}\right)$

(2) Obtain $x_k = x$, $z_k = z$, $w_k = w$ as the numerical solution of the nonlinear system

$$\begin{pmatrix} F_1(x) - b \\ Q_1^*(x - h\beta_0 w) - a_k \\ DF_1(x)Q_1 w + DF_1(x)Q_2 v \\ A(x)Q_1 w + A(x)Q_2 v + B(x)z + G(x) \end{pmatrix} = 0$$

The comments following algorithm 1 apply again; in particular, the nonlinear system in step (2) has to be solved with an error not exceeding $O(h^{\upsilon+1})$.

These results can be readily carried over to second order systems of the form (4.17). For this we assume now that the hypotheses of Theorem 6 are satisfied and hence that the existence of a solution $x: J \to E_x$, $z:J \to E_z$ of (4.17) is guaranteed which satisfies the initial conditions $x(0) = x_0$, $x'(0) = y_0$, $x''(0)=\eta(x_0,y_0)$, $z(0) = \zeta(x_0,y_0)$ for a given point $(x_0,y_0) \in E_x \times (E_y \cap \ker DF_1(x_0))$.

As above, let $x_c = x(t_c) \in M_b$, $b = F_1(x_0)$, be a current point on this solution where we construct a local parametrization (5.4) defined by the linear maps Q_1, Q_2. In section 5 we saw that in some neighborhood of x_c, where this parametrization is valid , the functions

(7.10) $$u = Q_1^*(x-x_c),\ v = Q_1^* x' .$$

satisfy the ODE (5.14).

In the second order case, the multistep method (7.3) now reads

(7.11a) $$u_k = \sum_{i=1}^{p} \alpha_i u_{k-i} + \sum_{i=0}^{p} \beta_i v'_{k-i},\ v_k = \sum_{i=1}^{p} \alpha_i v_{k-i} + \sum_{i=0}^{p} \beta_i v'_{k-i},$$

where

(7.11b) $$v'_i = Q_1^* \eta(\Phi(u_i), D\Phi(u_i)v_i).$$

As we saw at the end of section 5, v_i' is obtained by solving the linear system (5.15).

We begin again with the case $\beta_0 = 0$ and use the same notation and assumptions as before. In particular, let

(7.12) $$x_i \cong x(t_i),\ y_i \cong x'(t_i),\ w_i \cong \eta(x_i, y_i),\ z_i \cong z(t_i),\ i = 1,2,\ldots,k-1$$

be known approximations. Then we obtain the following the explicit-integration algorithm for computing from the last p points of this sequence the next approximate point:

<u>Algorithm 3.</u>

(1) Evaluate $a_k = Q_1^*(\sum_{i=1}^{p} \alpha_i x_{k-i} + h\sum_{i=1}^{p} \beta_i y_{k-i})$, $a'_k = Q_1^*(\sum_{i=1}^{p} \alpha_i y_{k-i} + h\sum_{i=1}^{p} \beta_i w_{k-i})$

(2) Solve the nonlinear system

$$\begin{pmatrix} F_1(x) - b \\ Q_1^* x - a_k \\ Q_1^* y - a'_k \\ DF_1(x)y \end{pmatrix} = 0$$

to obtain $x_k=x$, $y_k=y$.

(3) With $x=x_k$, $y=y_k$ obtain $w_k = Q_1\eta_1$ and $z_k = z$ as solutions of the linear system (5.15).

When $\beta_0 \neq 0$ then, analogous to algorithm 2, we can implement the multistep method (7.11a/b) for the numerical solution of (4.17) as follows:

<u>Algorithm 4.</u>

(1) Evaluate a_k,a'_k as in step (1) of algorithm 3.
(2) Solve the nonlinear system

$$\begin{pmatrix} F_1(x) - b \\ Q_1^*(x-\beta_0 hy) - a_k \\ Q_1^*(y-\beta_0 hw) - a'_k \\ DF_1(x)y \\ DF_1(x)Q_1\eta_1+DF_1(x)Q_2\eta_2 + D^2F_1(x)(y,y) \\ A(x,y)Q_1\eta_1+A(x,y)Q_2\eta_2+B(x,y)z + G(x,y) \end{pmatrix} = 0$$

to obtain $x_k=x$, $y_k=y$, $w_k= Q_1\eta_1$, $z_k=z$.

Obviously the comments made immediately following algorithm 1 apply again to both algorithm 3 and 4.

8. Application to the Euler-Lagrange Equations.

A classical example for second order DAEs of the form (4.17) are, of course, the equations arising in constrained multibody dynamics. These equations have the general form

$$\text{(8.1)} \qquad \begin{aligned} &\Psi(q,t) &&= 0, \\ &M(q,t)\, q'' + D_q\Psi(q,t)^T z + K(q,q',t) &&= 0, \end{aligned}$$

and are subsumed under the special case of (4.17) when both A and B depend only on x. In fact, we need to set only $x=(q,t)$ and define

$$\text{(8.2)} \qquad \begin{aligned} &F_1(x) = \Psi(q,t), \quad A(x) = \begin{pmatrix} M(q,t) & 0 \\ 0 & 1 \end{pmatrix}, \\ &B(x) = \begin{pmatrix} D_q\Psi(x,t)^T \\ 0 \end{pmatrix}, \quad G(x,x') = \begin{pmatrix} K(q,q',t) \\ 0 \end{pmatrix} \end{aligned}$$

Suppose that in (8.1) the mappings $\Psi: R^{n-1}\times R^1 \to R^r$, $K:(R^{n-1})^2\times R^1 \to R^{n-1}$, and $M:R^{n-1}\times R^1 \to L(R^{n-1},R^{n-1})$, $r < n-1$, satisfy, for all (q,t) under consideration, the smoothness conditions corresponding to (4.12a). Evidently, (4.12b) is here equivalent with

$$\text{(8.3)} \qquad \operatorname{rank} D_q\Psi(q,t) = r, \quad a^T M(q,t) a \neq 0, \ \forall\, a \in \ker D_q\Psi(q,t);$$

that is, with the assumptions that the algebraic constraints are independent and that the mass matrix M is definite on the nullspace of $D_q\Psi$. Thus, Theorem 6 applies to (8.1). Note also that now the defining relations (4.19) for the mappings $\eta:(R^{n-1})^2 \to R^{n-1}$, $\zeta: (R^{n-1})^2 \to R^r$, have the form

(8.4)

$$\begin{pmatrix} \eta(q,q',t) \\ \zeta(q,q',t) \end{pmatrix} = -\begin{pmatrix} M(q,t) & D_q\Psi(q,t)^T \\ D_q\Psi(q,t) & 0 \end{pmatrix}^{-1} \begin{pmatrix} K(q,q',t) \\ D^2_{qq}\Psi(q,t)(q',q')+2D^2_{qt}\Psi(q,t)q'+D^2_{tt}\Psi(u,t) \end{pmatrix}$$

We reduce (8.1) to a system of ODEs by using a local parametrizations of the type considered in section 6. However in doing so care should be taken not to modify the "special" variable t. By (8.2) we have

$$(8.5) \qquad DF_1(x) = (D_q\Psi(q,t),\ D_t\Psi(q,t)) \qquad .$$

and because of (8.3) there exist always r linearly independent columns among the first n-1 columns of $DF_1(x)$. Hence, when we construct a local parametrization by "coordinate partitioning" at a current point $x_c = (q_c,t_c)$ then we can always choose a permutation $j_1,...,j_{n-1}$ of the set $\{1,2,...,n-1\}$ such that the matrices

$$(8.6) \qquad Q_1 = (e_{j_{r+1}}, ..., e_{j_{n-1}}, e_n) = \begin{pmatrix} P_1 & 0 \\ 0 & 1 \end{pmatrix}, \quad Q_2 = (e_{j_1}, ..., e_{j_r}) = \begin{pmatrix} P_2 \\ 0 \end{pmatrix}$$

satisfy (5.3) and (6.2) and hence define the desired parametrization. Evidently, in (8.6) the $(n-1)\times r$ matrix P_1 and the $(n-1)\times(n-1-r)$ matrix P_2 consist of the basis vectors of R^{n-1} with indices $j_1,...,j_r$ and $j_{r+1},...,j_{n-1}$, respectively. In other words, we construct the parametrization (8.6) by working only with the $r\times(n-1)$ matrix $D_q\Psi(q_c,t_c)$ rather than with the $r\times n$ matrix $DF_1(x_c)$.

Analogously we can implement a "tangent space parametrization " by performing a QR-factorization of $D_q\Psi(q_c,t_c)^*$ rather than of $DF_1(x_c)^*$. More specifically, if

$$(8.7) \qquad D_q\Psi(q_c,t_c)^* = P\begin{pmatrix} R \\ 0 \end{pmatrix}$$

where P is an (n-1)-dimensional unitary matrix while R is again $r\times r$ upper-triangular, then, corresponding to (6.6), the matrices

$$(8.8) \quad Q_1 = \begin{pmatrix} P & 0 \\ 0 & 1 \end{pmatrix}(e_{r+1}, \dots, e_{n-1}, e_n) = \begin{pmatrix} P_1 & 0 \\ 0 & 1 \end{pmatrix}, \; Q_2 = \begin{pmatrix} P & 0 \\ 0 & 1 \end{pmatrix}(e_1, \dots, e_r) = \begin{pmatrix} P_2 \\ 0 \end{pmatrix}$$

satisfy (5.3) and (6.2) and hence define the desired parametrization. In (8.8), P_2 is the $(n-1)\times r$ matrix consisting of the first r columns of P, and the remaining (n-1-r) columns of P make up the $(n-1)\times(n-1-r)$ matrix P_1.

Now, the algorithms 3 and 4 of section can be applied. However since the matrices Q_1 ,Q_2 of (8.6) or (8.8) have a special form some simplifications are possible. Moreover, it should be taken into account that in many applications involving the equations (8.1) the accelerations

$$(8.9) \qquad x'' = \begin{pmatrix} q'' \\ 0 \end{pmatrix} = \eta(x, x')$$

are explicitly required.

Suppose again that the approximate points

$$x_i = (q_i, t_i), \ \ y_i = (q'_i, 1), \ \ w_i = (q''_i, 0), \ \ z_i \, , t_i = ih, \quad i=0,1,\ldots,k\text{-}1$$

are already known and that $x_c = (q_c, t_c)$ is the current point for the local parametrization. Note that the multistep method (7.11a/b) was assumed to be consistent so that, besides (7.4), the coefficients must satisfy

$$-\sum_{j=1}^{p} j\alpha_j + \sum_{j=0}^{p} \beta_j = 1$$

Hence, in step (2) of algorithm 3 and 4, the last equation of $Q_1^* x = a_k$ reduces to $t = kh$ while the last equation of $Q_1^* y = a'_k$ is trivially satisfied. Thus, the explicit algorithm 3 can be simplified as follows:

<u>Algorithm 5.</u>

(1) Evaluate $a_k = P_1^*(\sum_{i=1}^{p} \alpha_i q_{k-i} + h\sum_{i=1}^{p} \beta_i q'_{k-i}), \ \ a'_k = P_1^*(\sum_{i=1}^{p} \alpha_i q'_{k-i} + h\sum_{i=1}^{p} \beta_i q''_{k-i})$

(2) Obtain $q_k = q$, $q'_k = q'$ as solutions of the nonlinear system

$$\begin{pmatrix} \Psi(q,t_k) \\ P_1^* q - a_k \\ P_1^* q' - a'_k \\ D_q\Psi(q,t_k)q' + D_t\Psi(q,t_k) \end{pmatrix} = 0$$

(3) With $q=q_k$, $q'=q'_k$ solve the linear system (8.4) to obtain $q"_k = q"$, and $z_k = z$

For the implicit algorithm, it is useful to introduce the abbreviation

$$\gamma(q,q',t) = -D^2_{qq}\Psi(q,t)(q',q') - 2D^2_{qt}\Psi(q,t)q' - D^2_{tt}\Psi(q,t).$$

Then, with the acceleration (8.9), the last equations in the nonlinear system of step 2 of algorithm 4 can be written in the form

$$D_q\Psi(q, t_k)q" = \gamma(q, q', t_k)$$
$$M(q, t_k)q" + D_q\Psi(q, t_k)^T z + K(q, q', t_k) = 0$$

Evidently, the first of these equations can also be obtained formally by differentiating the first equation of (8.1) twice.

With these observations , algorithms 4 reduces to the following algorithm:

<u>Algorithm 6</u>.

(1) Evaluate a_k, a'_k as in step (1) of algorithm 5.

(2) Obtain $q_k=q$, $q'_k=q'$, $q"_k= q"$, $z_k=z$ as solution of the nonlinear system

$$\begin{pmatrix} \Psi(q, t_k) \\ P_1^*(q-\beta_0 hq') - a_k \\ P_1^*(q'-\beta_0 hq") - a'_k \\ D_q\Psi(q, t_k)q' + D_t\Psi(q, t_k) \\ D_q\Psi(q, t_k)q" + \gamma(q,q',t_k) \\ M(q,t_k)q"+D_q\Psi(q, t_k)^T z + K(q,q',t_k) \end{pmatrix} = 0$$

The numerical solution of the nonlinear system (9.23) represents a significant computational challenge. However, in a separate paper it shall be shown that when proper care is taken to exploit its special structure, then the computational complexity of this problem can be reduced greatly.

10. A numerical example

A frequently encountered basic mechanisms is the four-bar system shown schematically in Figure 1. To model this system, each of the four links and the ground are considered as a body and marked by the integers 1, 2, 3, 4. A frame is fixed for each body with the origin at its centroid. For each body the coordinates of the centroid are given in Table 1. This identifies also the initial position of the system as it is sketched in Figure 1. Table 2 lists the mass and moment of inertia for each body. All the joints of the mechanism are revolute joints, they are marked by the letters A, B, C, D. Table 3 identifies the two bodies connected at each joint and gives the coordinates of the common point in the coordinate frame of each body. . The mechanism is subject to no applied force other than gravity. The initial velocity of each generalized coordinate is assumed to be equal to zero.

Body #	1	2	3	4
x	0.0	2.0	6.0	12.0
y	0.0	2.0	4.0	4.0
θ	0.0	$\pi / 4$	0.0	$\pi / 4$

Table 1 : Body centroids

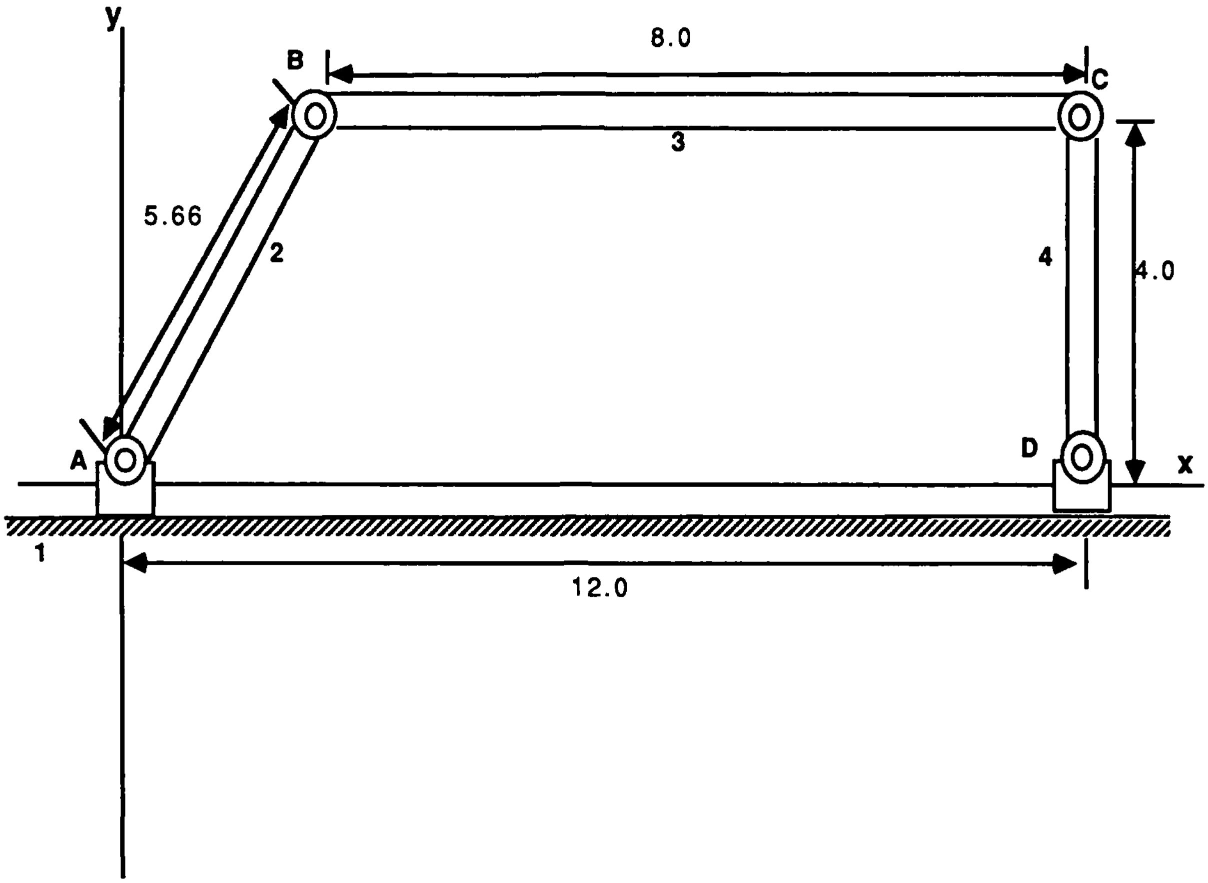

Figure 1: Fourbar-Linkage

Body #	1	2	3	4
Mass (kg)	1.0	200.0	300.0	100.0
Inertia $(kgm)^2$	1.0	200.0	300.0	100.0

Table 2: Masses and Moments of Inertia

Joint	A	B	C	D
Body i	1	2	3	4
$x_i(P)$	0.0	2.828	4.0	2.0
$y_i(P)$	0.0	0.0	0.0	0.0
Body j	2	3	4	1
$x_j(P)$	-2.828	-4.0	-2.0	12.0
$y_j(P)$	0.0	0.0	0.0	0.0

Table 3: Joint data at the common point P

The constrained equations of motion for this system have been solved using the algorithms discussed in Section 9. At the same time, as a check the model was also analyzed by means of DADS, a general purpose code for mechanical design [2].

The numerical experiments were carried out with the implicit as well as the explicit algorithm. The second order BDF-formula was chosen as the implicit method and the second order PECE- (Adams -Bashforth - Moulton)-formula as the explicit method. In each case, fixed-stepsizes h=0.01, and h=0.0025 were applied. The nonlinear systems were solved by a chord Newton method. As indicated earlier, the local parametrization was changed whenever the estimated condition number of the linear systems exceeded a specific bound or when the nonlinear solver failed to converge in a given number of steps. In Figures 2-4 we show the position, velocity, and acceleration of the x-coordinate of the centroid of body 2 for the tangent space parametrization.

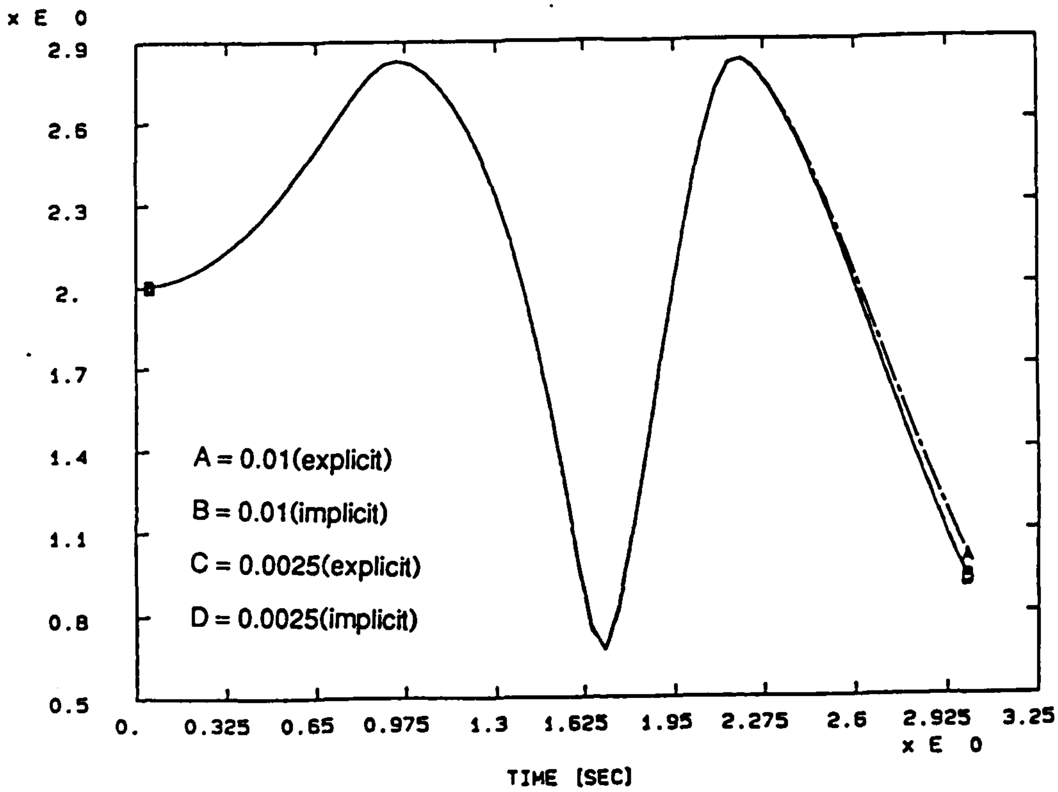

Figure 2: Position of the x-coordinate of the centroid of body 2.

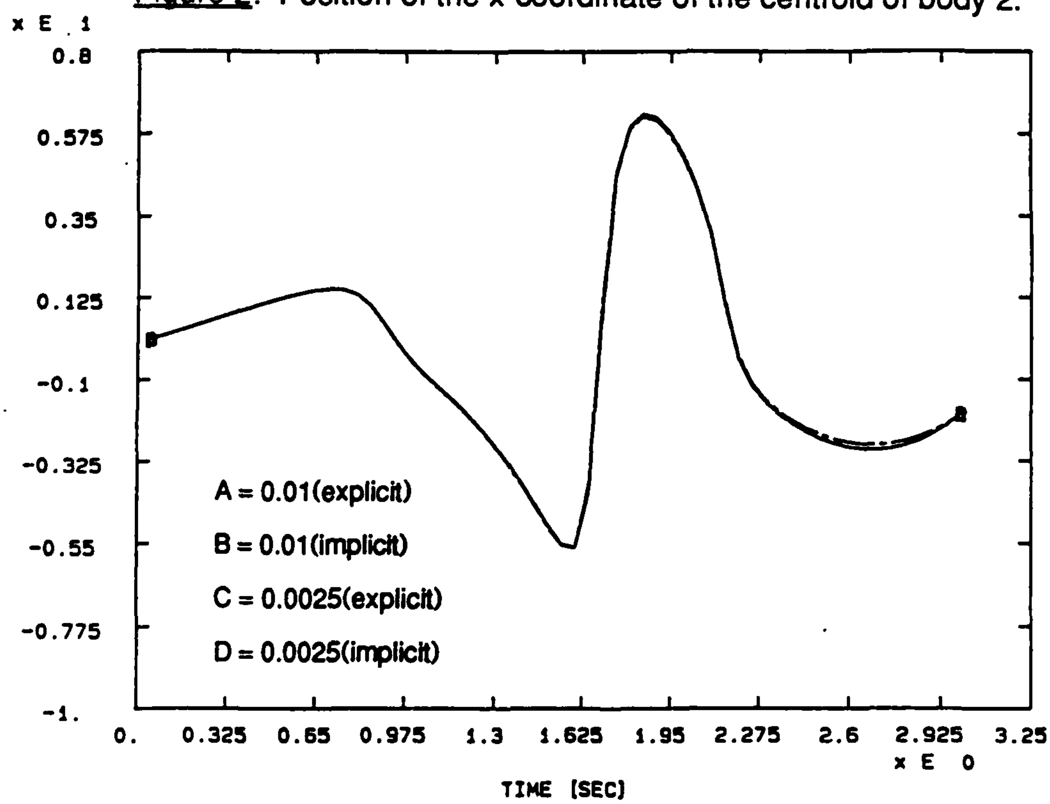

Figure 3. Velocity of the x-coordinate of the centroid of body 2.

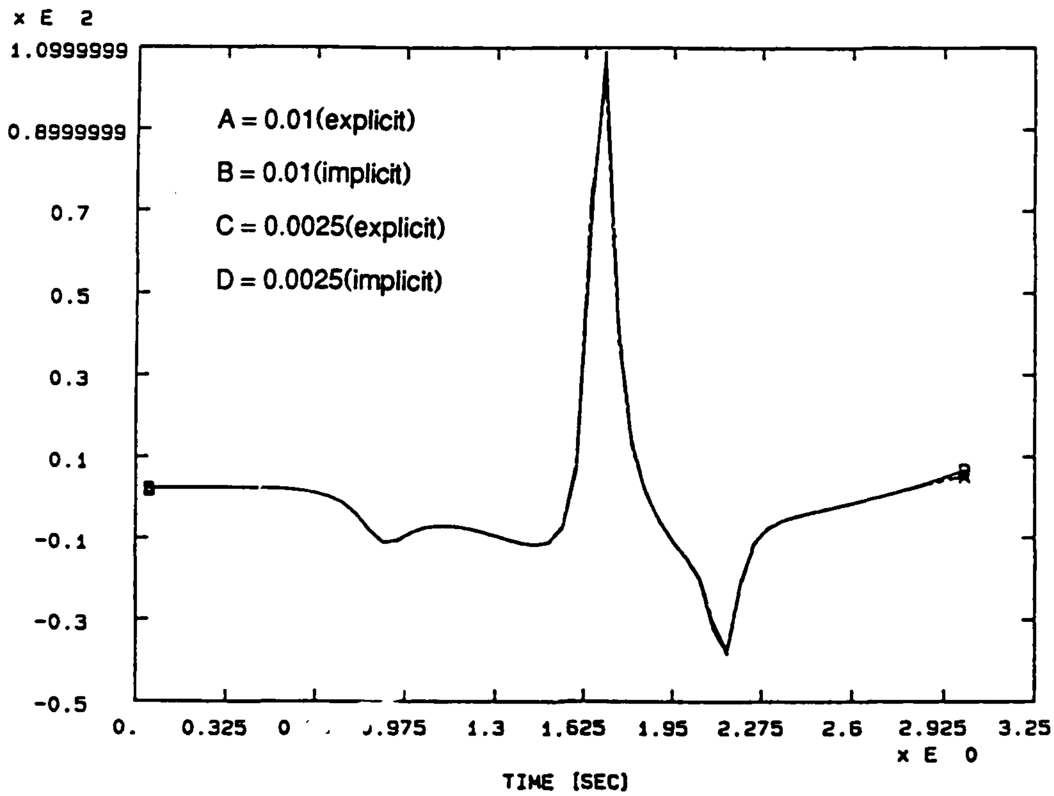

Figure 4: Acceleration of the x-coordinate of the centroid of body 1.

The numerical solutions obtained with the implicit method are accurate to four decimal digits throughout the time interval [0,3] and hence, in the figures, they cannot be distinguished from the solutions given by DADS. On the other hand, the solutions obtained with the explicit method are drifting away for $t >$ 2.5 sec. (see Fig 2, 3, 4) when the the stepsize is increased.

The computations were also carried out with the local parametrization, induced by "coordinate partitioning " and they agree to three significant digits with the result for the "tangent space" parametrization. Table 4 provides some statistical information about the total number of function and Jacobian evaluations as well as about the number of re-parametrizations for the two choices of local parametrizations when the step-size $h = 0.01$ was used. In the table, TG and GCP stands for the tangent space and coordinate partitioning parametrization, respectively.

	Explicit Method		Implicit Method	
	TG	GCP	TG	GCP
Function Eval.	989	1021	1456	1520
Jacobian Eval.	56	65	134	153
Re-Parametr.	6	6	15	19

Table 4 : Performance Statistics

Acknowledgement: We would like to thank Mr. Jeng Yen for helping us with many of the numerical experiments.

References

[1] K.Brennan, S.Campbell, L.Petzold, Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations,North-Hollond,New-York,1989

[2] DADS User's Manual , Rev. 4.0, Computer Aided Design Software, Inc., Oakdale, Iowa,1987.

[3] G.H.Golub, C.F.VanLoan, Matrix Computations, Johns Hopkins Univ. Press, Baltimore,MD 1983

[4] E. Griepentrog, R. Maerz, Differential-Algebraic Equations and Their Numerical Treatment, B.G.Teubner Verlag, Leipzig, 1986

[5] E.J.Haug,J.Yen, Implicit Numerical Integration of Constrained Equations of Motion via Generalized Coordinate Partitioning , Univ. of Iowa, Ctr. for Simulation and Design Optim. of Mech. Systems, Tech. Rep. R-39, Feb. 1989

[6] S.Lang, Introduction to Differentiable Manifolds, Wiley , New York, NY, 1962

[7] J.M. Ortega, W.C.Rheinboldt, Iterative Methods for Nonlinear Equations in Several Variables, Academic Press, New York, 1970

[8] F.A.Potra, J.Yen, Implicit Numerical Integration for Euler-Lagrange Equations via Tangent Space Parametrization, Univ. of Iowa, Ctr. for Simulation and Design Optim. of Mech. Systems, Tech. Rep. R-56, June 1989

[9] S.Reich, Beitraege zur Theorie der Algebrodifferentialgleichungen, Ph.D. Dissertation (Electronics), Techn. Univ. Dresden, Spring 1988

[10] W. C. Rheinboldt, Di rential-Algebraic Systems as Differential Equations on Manifolds, Math. of Comp. 43, 1984, 473-482

[11] W.C. Rheinboldt, Numerical Analysis of Parametrized Nonlinear Equations, John Wiley and Sons, New York, 1986

[12] W.C.Rheinboldt, On the Existence and Computation of Solutions of Nonlinear Semi-Implicit Algebraic Equations, University of Pittsburgh, Inst. f. Comp. Math. and Appl., Tech. Rep. ICMA-89-139, August 1989; SIAM J. Num. Anal., submitted

[13] M Spivak, A Comprehensive Introduction to Differential Geometry, Vol 1-5, Publish or Perish, Inc. Boston, MA 1970